A General Discussion
on

Time-Resolved Chemistry: From Structure to Function

A General Discussion on Time-Resolved Chemistry was held at the University of Manchester, UK on 24th, 25th and 26th June, 2002.

Contents

1 Introductory Lecture: Time-resolved chemistry at atomic resolution
Philip Coppens and **Irina V. Novozhilova**

13 The realization of sub-nanosecond pump and probe experiments at the ESRF
Michael Wulff, Anton Plech, Laurent Eybert, Rudolf Randler, Friedrich Schotte and **Philip Anfinrud**

27 Femtosecond mid-infrared spectroscopy of condensed phase hydrogen-bonded systems as a probe of structural dynamics
Matteo Rini, Andreas Kummrow, Jens Dreyer, Erik T. J. Nibbering and **Thomas Elsaesser**

41 What we can learn about fast chemical processes from slow diffraction experiments
Hans-Beat Bürgi

65 The frontiers of time-resolved macromolecular crystallography: movies and chirped X-ray pulses
Keith Moffat

79 General Discussion

89 Achieving photo-control of protein conformation and activity: producing a photo-controlled leucine zipper
Janet R. Kumita, Daniel G. Flint, G. Andrew Woolley and **Oliver S. Smart**

105 First investigations of the kinetics of the topochemical reaction of *p*-formyl-*trans*-cinnamic acid by time-resolved X-ray diffraction
G. Busse, T. Tschentscher, A. Plech, M. Wulff, B. Frederichs and **S. Techert**

119 Nanosecond time-resolved crystallography of photo-induced species: case study and instrument development for high-resolution excited-state single-crystal structure determination
Jacqueline M. Cole, Paul R. Raithby, Michael Wulff, Friedrich Schotte, Anton Plech, Simon J. Teat and **Graham Bushnell-Wye**

131 Time-resolved and static-ensemble structural chemistry of hydroxymethylbilane synthase
John R. Helliwell, Yeu Perng Nieh, Jarjis Habash, Paul F. Faulder, James Raftery, Michele Cianci, Michael Wulff and **Alfons Hädener**

145 Structural dynamics of the receptor-binding domain of colicin E9
Ruth Boetzel, Emily S. Collins, Nigel J. Clayden, Colin Kleanthous, Richard James and **Geoffrey R. Moore**

163 The dynamic transition in proteins may have a simple explanation
Roy M. Daniel, John L. Finney and **Jeremy C. Smith**

This journal is © The Royal Society of Chemistry 2002

171 General Discussion

191 Mechanism of formation of DNA–cationic vesicle complexes
Paula C. A. Barreleiro, Roland P. May and **Björn Lindman**

203 Following the formation of nanometer-sized clusters by time-resolved SAXS and EXAFS techniques
Florian Meneau, Gopinathan Sankar, Norberto Morgante, Rudolf Winter, C. Richard A. Catlow, G. Neville Greaves and **John Meurig Thomas**

211 Application of stopped flow techniques and energy dispersive EXAFS for investigation of the reactions of transition metal complexes in solution: Activation of nickel β-diketonates to form homogeneous catalysts, electron transfer reactions involving iron(III) and oxidative addition to iridium(I)
M. Basyaruddin B. Abdul Rahman, Peter R. Bolton, John Evans, Andrew J. Dent, Ian Harvey and **Sofia Diaz-Moreno**

223 Direct dynamics calculations of reaction rate and kinetic isotope effects in enzyme catalysed reactions
Gary Tresadern, Sara Nunez, Paul F. Faulder, Hong Wang, Ian H. Hillier and **Neil A. Burton**

243 Time-resolved computational protein biochemistry: Solvent effects on interactions, conformational transitions and equilibrium fluctuations
Alexander L. Tournier, Danzhi Huang, Sonja M. Schwarzl, Stefan Fischer and **Jeremy C. Smith**

253 Theoretical studies of time-resolved spectroscopy of protein folding
Jonathan D. Hirst, Samita Bhattacharjee and **Alexey V. Onufriev**

269 General Discussion

283 Chemistry, physics and time: the computer modelling of glassmaking
David Martlew

299 A SAXS/WAXS XAFS study of crystallisation in cordierite glass
G. N. Greaves, W. Bras, M. Oversluizen and **S. M. Clark**

315 Excited state molecular structure determination in disordered media using laser pump/X-ray probe time-domain X-ray absorption spectroscopy
Lin X. Chen

331 Recent results from the *in situ* study of hydrothermal crystallisations using time-resolved X-ray and neutron diffraction methods
Richard I. Walton, Alexander Norquist, Ronald I. Smith and **Dermot O'Hare**

343 Are metastable, precrystallisation, density-fluctuations a universal phenomena?
Ellen L. Heeley, C. Kit Poh, Wu Li, Anna Maidens, Wim Bras, Igor P. Dolbnya, Anthony J. Gleeson, Nicolas J. Terrill, J. Patrick A. Fairclough, Peter D. Olmsted, Rile I. Ristic, Micheal J. Hounslow and **Anthony J. Ryan**

363 *In situ* neutron diffraction studies of single crystals and powders during microwave irradiation
Andrew Harrison, Richard Ibberson, Graeme Robb, Gavin Whittaker, Chick Wilson and **Douglas Youngson**

381 General Discussion

395 Concluding Remarks: Time-resolved chemistry: from structure to function. A summary
John Meurig Thomas

401 List of Posters

403 List of Participants

405 Index of Contributors

This journal is © The Royal Society of Chemistry 2002